Solution for Problem 27

Chem 540

(1) The wavefunction for a particle in a box is

$$\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right).$$

Thus

$$\langle x \rangle = \int \overline{\psi(x)} x \psi(x)\, dx = \frac{2}{L}\int_0^L x \sin^2\left(\frac{n\pi x}{L}\right) dx = \frac{L}{2}$$

and

$$\left\langle x^2 \right\rangle = \int \overline{\psi(x)} x^2 \psi(x)\, dx = \frac{2}{L}\int_0^L x^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = \frac{L^2}{3} - \frac{L^2}{2n^2\pi^2}$$

For the last calculation the code is:

```
\[Psi][x_] := Assuming[n \[Element] Integers, Sqrt
    [2/L] Sin[n Pi x/L]]
Assuming[n \[Element] Integers, Integrate[x^2*\[Psi
    ][x]^2, {x, 0, L}]] // FullSimplify
```

(2) For the moments of momenta, we have:

$$\begin{aligned}
\langle p \rangle &= \int_0^L \overline{\psi(x)} (-i\hbar)\, \partial_x \psi(x)\, dx = \\
&= -\frac{2i\hbar}{L}\int_0^L dx\ \sin\left(\frac{n\pi x}{L}\right)\cos\left(\frac{n\pi x}{L}\right)\frac{n\pi}{L} \\
&= -\frac{i\hbar n\pi}{L^2}\int_0^L \sin\left(\frac{2n\pi x}{L}\right) dx = 0
\end{aligned}$$

and

$$\begin{aligned}
\langle p \rangle &= \int_0^L \overline{\psi(x)} (-i\hbar)^2\, \partial_{x,x} \psi(x)\, dx \\
&= +\frac{2\hbar^2}{L}\left(\frac{n\pi}{L}\right)^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx \\
&= +\frac{2\hbar^2}{L}\left(\frac{n\pi}{L}\right)^2 \frac{L}{2} = \frac{\hbar^2 n^2 \pi^2}{L^2}
\end{aligned}$$

Inside the box, the potential is zero, so

$$\frac{\hat{p}^2}{2m}\psi(x) = E\psi(x)$$

Therefore, we must have that

$$\left\langle p^2 \right\rangle = 2m \langle E \rangle$$

But we know from solving the Schrodinger equation for this system that $E_n = n^2h^2/8mL^2 = n^2\hbar^2\pi^2/2mL^2$. From the above relation, $\left\langle p^2 \right\rangle = n^2\hbar^2\pi^2/L^2$, precisely the value we obtained from explicit calculation of the second moment.

(3) The uncertainties in position and momentum are

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = L\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}$$

and

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \frac{n\hbar\pi}{L},$$

respectively. Therefore their product is

$$\begin{aligned} \Delta x \Delta p &= n\hbar\pi\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}} \\ &= \hbar\sqrt{\frac{n^2\pi^2}{12} - \frac{1}{2}} \end{aligned}$$

Observe that the quantity under the square root is an increasing function of the *integer* n, therefore, the smallest value of $\Delta x \Delta p$ will be attained when $n = 1$:

$$\min(\Delta x \Delta p) = \hbar\sqrt{\frac{\pi^2}{12} - \frac{1}{2}} \simeq 0.57\hbar \geq \hbar/2$$

Therefore, $\Delta x \Delta p \geq \hbar/2, \forall n \in \mathbb{N}$.